

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-  
163702-07-6 | DTXSID4073120

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 1.32e-14 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.62e-01

**Confidence level:** 6.76e-01

## Nearest Neighbors from the Training Set

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Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-

**Measured:** 7.20e-15

**Predicted:** 1.32e-14

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Propane, 1,1,1,2,2,3,3-heptafluoro-3-methoxy-

**Measured:** 1.18e-14

**Predicted:** 1.85e-14

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

**Measured:** 1.12e-13

**Predicted:** 6.54e-14

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Heptafluoroisopropyl methyl ether

**Measured:** 1.52e-14

**Predicted:** 2.77e-14

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HFE-347pcf2

**Measured:** 9.40e-14

**Predicted:** 6.55e-14